Thioacetamide 62-55-5 | DTXSID9021340

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Marada I	D. L.
Model	Data
110001	Bata

Weighted KNN model

5-fold CV (75%)		Training (75	Training (75%)		Test (25%)		
Q2	RMSE	R2	RMSE	R2	RMSE		
0.85	0.69	0.86	0.67	0.86	0.78		

Model Results

Predicted value: -0.157

Global applicability domain: Inside

Local applicability domain index: 4.91e-01

Confidence level: 7.06e-01

Nearest Neighbors from the Training Set

Image not found

Thioacetamide

Measured: -0.260

Predicted: -0.157

Image not found

Cyclopropanecarbonitrile

Measured: 0.68 Predicted: 5.50e-01

Image not found

Cyclopropane carboxylic acid

Measured: 0.63 Predicted: 5.47e-01

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Methacrylamide Measured: -1.11 Predicted: -0.868

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Propionitrile

Measured: 0.16

Predicted: 2.18e-01